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SHORT COMMUNICATION

Draft GUM Supplement 1 and Bayesian analysis

Clemens Elster[1], **Wolfgang Wöger**[2] **and Maurice G Cox**[3]

[1] Physikalisch-Technische Bundesanstalt, Abbestrasse 2-12, 10587 Berlin, Germany
[2] Drosselweg 1, 50735 Köln, Germany[4]
[3] National Physical Laboratory, Teddington, Middlesex TW11 0LW, UK

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Abstract
The relation between uncertainty evaluation according to the recent draft of GUM Supplement 1 and the application of Bayesian statistics including Bayes' theorem is considered. In the case of a Type A evaluation of uncertainty, repeated measurement indications are regarded as independently drawn from normal frequency distributions and, according to its suggestion, the numerical evaluation method of Supplement 1 is applied *after* having assigned scaled and shifted t-distributions to the corresponding input quantities. It will be shown that this approach is equivalent to a Bayesian analysis using Bayes' theorem with commonly used prior distributions.

The recent draft of GUM Supplement 1 [1] treats the numerical calculation of measurement uncertainty by a Monte Carlo method (MCM) as an implementation of the propagation of distributions. It applies to the situation where the relation between input quantities $X_1, \ldots, X_N$ and the measurand Y is stated in terms of a model

$$Y = f(X_1, \ldots, X_N) \tag{1}$$

(as in the GUM [2]), and a joint probability density function (PDF) $g_{X_1,\ldots,X_N}(\xi_1, \ldots, \xi_N)$ is available that expresses the knowledge about the input quantities $X_1, \ldots, X_N$.

Supplement 1 specifies the application of MCM to obtain numerically an estimate y of Y and the standard uncertainty associated with y, as well as coverage intervals for Y for specified coverage probabilities. The calculations are based on the numerical determination of a PDF for Y. Advantages of the approach are that (a) the model (1) is fully taken into account, in contrast to the GUM [2], which uses a linear approximation to the model, and (b) coverage intervals are determined without making a distributional assumption.

For many practical situations, corresponding to independent input quantities X_i, the joint PDF factorizes into the product of PDFs individually for the X_i:

$$g_{X_1,\ldots,X_N}(\xi_1, \ldots, \xi_N) = g_{X_1}(\xi_1) \cdots g_{X_N}(\xi_N). \tag{2}$$

Supplement 1 provides a PDF $g_{X_i}(\xi_i)$ for X_i in some common situations. For instance, when the information about X_i consists of an estimate x_i and its associated standard uncertainty $u(x_i)$, by applying the principle of maximum entropy a Gaussian PDF with expectation x_i and standard deviation $u(x_i)$ is assigned to X_i. Regarding a Type A evaluation of uncertainty, Supplement 1 considers the case where, for single quantities, repeated measurement indications are available that are regarded as independently drawn from normal frequency distributions (each with unknown expectation and unknown variance). In this case scaled and shifted t-distributions are assigned, where the t-distribution describes the knowledge about the expectation of the according frequency distribution.

In this communication the relation between the Supplement 1 approach and the explicit application of Bayes' theorem in the framework of Bayesian statistics is considered in the following circumstances. In the case of repeated measurement indications of some of the input quantities, $X_1, \ldots, X_{N_A}$, say, all corresponding indications are considered as being obtained independently. Denote by $D_i = \{x_{i,1}, \ldots, x_{i,n_i}\}$ the set of indications corresponding to X_i (where $n_i \geqslant 4$). All indications in D_i are regarded as drawn from a normal distribution with unknown expectation (the value of X_i) and unknown variance σ_i^2. For the input quantities $X_{N_A+1}, \ldots, X_N$, information is encoded by the given

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[4] Formerly Physikalisch-Technische Bundesanstalt, Bundesallee 100, 38116 Braunschweig, Germany.

joint PDF $g_{X_{N_A+1},\dots,X_N}(\xi_{N_A+1},\dots,\xi_N)$, corresponding to Type B evaluations of uncertainty. For a Bayesian treatment, commonly used prior distributions are considered for those unknown parameters for which no information is given.

For ease of notation, let $X_1,\dots,X_N,Y$ also represent the unknown values of the corresponding quantities, $\boldsymbol{Z} = (X_1,\dots,X_{N_A},X_{N_A+1},\dots,X_N,\sigma_1^2,\dots,\sigma_{N_A}^2,Y)^{\mathrm{T}}$ the vector of all unknowns and $(\boldsymbol{\xi}^{\mathrm{T}},\eta)^{\mathrm{T}} = (\xi_1,\dots,\xi_{N_A},\xi_{N_A+1},\dots,\xi_N,\xi_{N+1},\dots,\xi_{N+N_A},\eta)^{\mathrm{T}}$ the possible values of these unknowns.

The Bayesian analysis starts with a prior PDF $g_{\boldsymbol{Z}}(\boldsymbol{\xi},\eta)$ expressing the knowledge about $\boldsymbol{Z}$ without reference to the data $\{D_1,\dots,D_{N_A}\}$. Application of Bayes' theorem,

$$g_{\boldsymbol{Z}}(\boldsymbol{\xi},\eta|\mathrm{data}) \propto \ell(\boldsymbol{\xi},\eta|\mathrm{data})g_{\boldsymbol{Z}}(\boldsymbol{\xi},\eta), \tag{3}$$

then yields a posterior PDF for $\boldsymbol{Z}$ after taking into account the data. In expression (3), $\ell(\boldsymbol{\xi},\eta|\mathrm{data})$ denotes the likelihood which is given here by

$$\ell(\boldsymbol{\xi},\eta|\mathrm{data}) = \prod_{i=1}^{N_A}\frac{1}{(2\pi\xi_{N+i})^{n_i/2}}\exp\left[-\frac{1}{2\xi_{N+i}}\sum_{\alpha=1}^{n_i}(\xi_i-x_{i,\alpha})^2\right]. \tag{4}$$

For the prior distribution,

$$g_{\boldsymbol{Z}}(\boldsymbol{\xi},\eta) = g_{X_1,\dots,X_N,Y}(\xi_1,\dots,\xi_N,\eta)\, g_{\sigma_1^2}(\xi_{N+1}) \cdots g_{\sigma_{N_A}^2}(\xi_{N+N_A}) \tag{5}$$

is considered with $g_{\sigma_i^2}(\xi_{N+i}) \propto 1/\xi_{N+i}, i = 1,\dots,N_A$ (often called a Jeffreys' prior), and

$$\begin{aligned} g_{X_1,\dots,X_N,Y}&(\xi_1,\dots,\xi_N,\eta) \\ &= g_{X_1,\dots,X_N}(\xi_1,\dots,\xi_N)g_{Y|X_1,\dots,X_N}(\eta|\xi_1,\dots,\xi_N) \\ &= g_{X_1,\dots,X_N}(\xi_1,\dots,\xi_N)\delta[\eta - f(\xi_1,\dots,\xi_N)]. \end{aligned} \tag{6}$$

In expression (6), the conditional PDF for Y given $X_1,\dots,X_N$ accounts for the stated model relation (1) and is given by the delta function $\delta[\eta - f(\xi_1,\dots,\xi_N)]$ (sometimes called the model prior [3]). This assignment ensures that only those $(\xi_1,\dots,\xi_N,\eta)$ are considered that satisfy the model relation (1). For the prior PDF $g_{X_1,\dots,X_N}(\xi_1,\dots,\xi_N)$, finally,

$$\begin{aligned} g_{X_1,\dots,X_N}&(\xi_1,\dots,\xi_N) \\ &= g_{X_1}(\xi_1)\cdots g_{X_{N_A}}(\xi_{N_A})\, g_{X_{N_A+1},\dots,X_N}(\xi_{N_A+1},\dots,\xi_N) \end{aligned} \tag{7}$$

is considered with $g_{X_1}(\xi_1) = \dots = g_{X_{N_A}}(\xi_{N_A}) \propto 1$ and $g_{X_{N_A+1},\dots,X_N}(\xi_{N_A+1},\dots,\xi_N)$ the given PDF for $X_{N_A+1},\dots,X_N$. Hence, the prior distribution $g_{\boldsymbol{Z}}(\boldsymbol{\xi},\eta)$ is constructed by utilizing the model relation (1), the given PDF $g_{X_{N_A+1},\dots,X_N}(\xi_{N_A+1},\dots,\xi_N)$ for $X_{N_A+1},\dots,X_N$, and the usual non-informative priors for $X_1,\dots,X_{N_A},\sigma_1^2,\dots,\sigma_{N_A}^2$.

The likelihood (4) and the prior (5), together with the PDFs (6) and (7), determine the posterior PDF $g_{\boldsymbol{Z}}(\boldsymbol{\xi},\eta|\mathrm{data})$ in expression (3), and the sought PDF $g_Y(\eta|\mathrm{data})$ is then obtained by marginalization:

$$\begin{aligned} g_Y(\eta|\mathrm{data}) &= \int g_{\boldsymbol{Z}}(\boldsymbol{\xi},\eta|\mathrm{data})\,\mathrm{d}\xi_1\dots\mathrm{d}\xi_{N+N_A} \\ &\propto \int \ell(\boldsymbol{\xi},\eta|\mathrm{data})g_{\boldsymbol{Z}}(\boldsymbol{\xi},\eta)\,\mathrm{d}\xi_1\dots\mathrm{d}\xi_{N+N_A}. \end{aligned} \tag{8}$$

By carrying out the integration in expression (8) with respect to the variance parameters $\sigma_1^2,\dots,\sigma_{N_A}^2$, N_A integrals of the form

$$\int_0^\infty \frac{1}{\xi_{N+i}^{1+n_i/2}}\exp\left[-\frac{1}{2\xi_{N+i}}\sum_{\alpha=1}^{n_i}(\xi_i - x_{i,\alpha})^2\right]\mathrm{d}\xi_{N+i} \tag{9}$$

are obtained, each of which equals (up to a normalization factor) a correspondingly scaled and shifted t-distribution with argument ξ_i [4]. (That is, $(\xi_i - \bar{x}_i)/(s_i/n_i^{1/2})$ follows a t_{n_i-1}-distribution with $\bar{x}_i$ and s_i denoting average and standard deviation of $D_i = \{x_{i,1},\dots,x_{i,n_i}\}$.) Hence, after marginalization with respect to the nuisance parameters $\sigma_1^2,\dots,\sigma_{N_A}^2$, the posterior PDF for Y reduces to the so-called Markov formula [5]

$$\begin{aligned} g_Y(\eta|\mathrm{data}) = \int & g_{X_1,\dots,X_N}(\xi_1,\dots,\xi_N)\delta[\eta - f(\xi_1,\dots,\xi_N)] \\ & \times\mathrm{d}\xi_1\dots\mathrm{d}\xi_N, \end{aligned} \tag{10}$$

where $g_{X_1,\dots,X_N}(\xi_1,\dots,\xi_N)$ is the product of N_A scaled and shifted t-distributions assigned to $X_1,\dots,X_{N_A}$ and the given PDF $g_{X_{N_A+1},\dots,X_N}(\xi_{N_A+1},\dots,\xi_N)$ associated with $X_{N_A+1},\dots,X_N$. Since formula (10) is the starting point of the Monte Carlo procedure in Supplement 1 [1], and since the PDF $g_{X_1,\dots,X_N}(\xi_1,\dots,\xi_N)$ is in accordance with the treatment of Supplement 1, the results obtained by Supplement 1 are those of a Bayesian analysis with commonly used priors.

In the absence of quantities the knowledge of which constitutes repeated measurement indications, there is no data and Bayes' theorem (3) cannot be applied. A Bayesian view would in this case yield the prior distribution (5) (with the terms corresponding to repeated measurement indications being omitted, i.e. $N_A = 0$) as the PDF for $\boldsymbol{Z}$, from which the PDF for Y is then determined by marginalization, again yielding the right-hand side of expression (10).

Recent work [6] indicated that for some problems of the type considered here there could be a difference between the results of applying the approach of Supplement 1 and a Bayesian treatment, in contrast to the conclusion here. This apparent divergence can, however, be attributed to the use of different priors in the Bayesian treatments here and in that paper.

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